

Understanding and mitigating droop in nitride LEDs

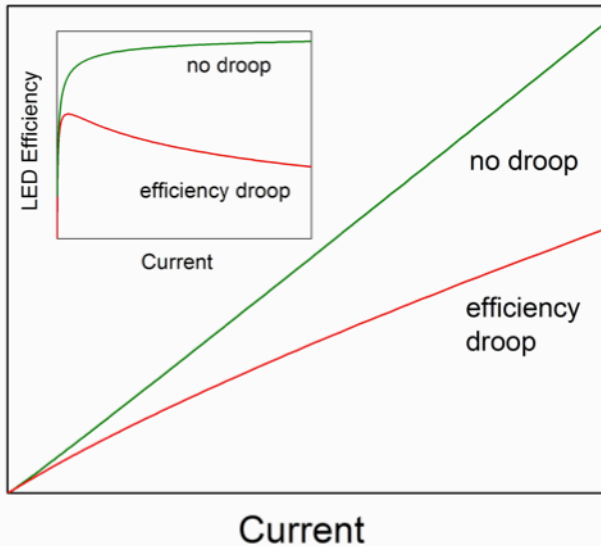
Emmanouil (Manos) Kioupakis

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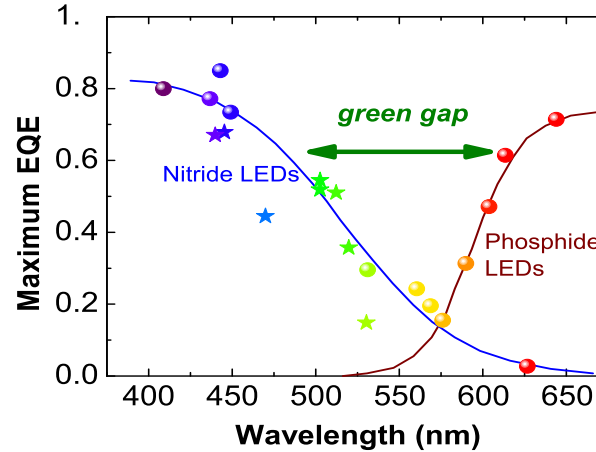


Challenges with nitride LEDs

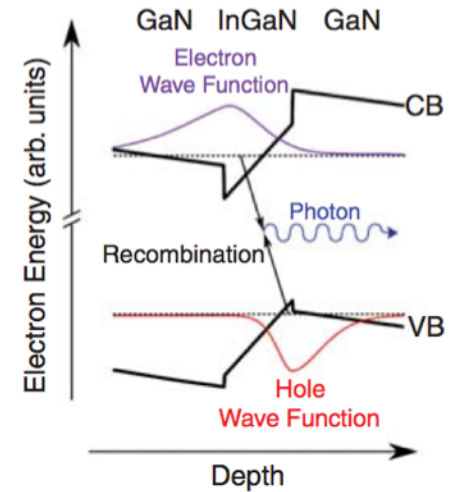
LED Light Power



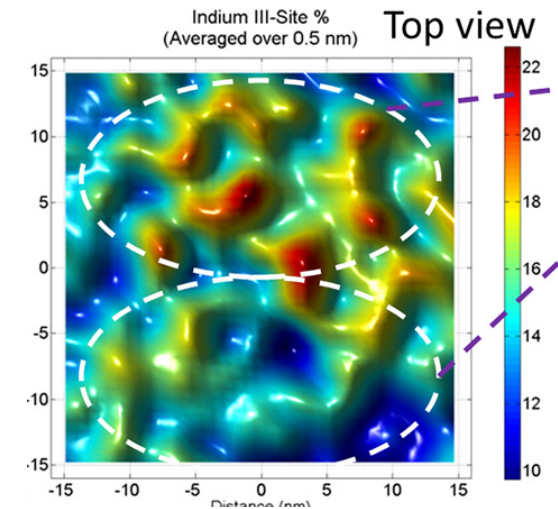
Piprek, *phys. status solidi (a)* **207**, 2217 (2010).



Auf Der Maur *et al.*, *Phys. Rev. Lett.* **116**, 027401 (2016).



Speck and Chichibu, *MRS Bull.* **34**, 304 (2009)

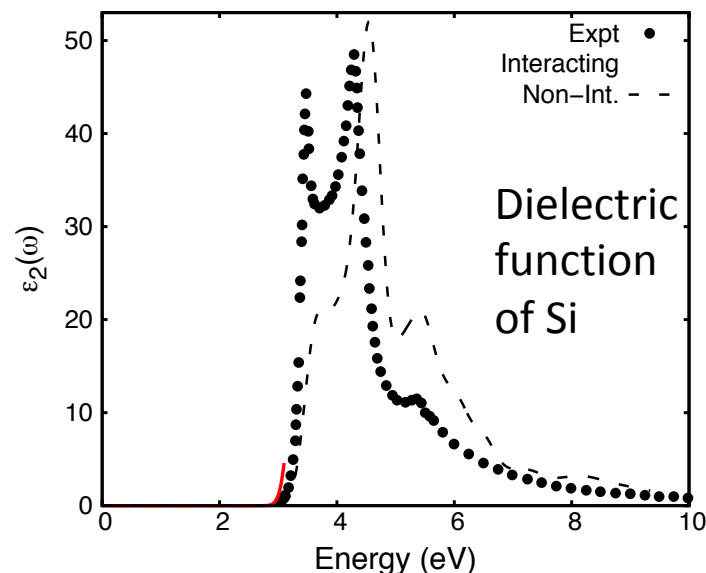
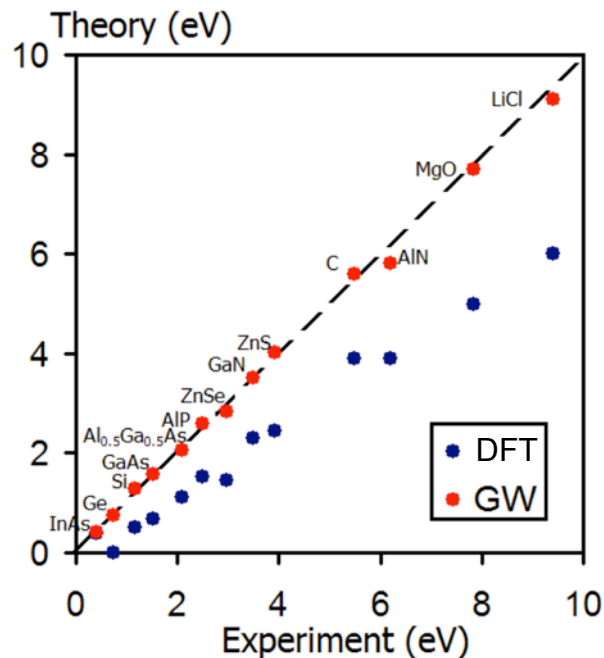


Wu *et al.*, *Appl. Phys. Lett.* **101**, 083505 (2012)

1. Droop: lower efficiency at high power
2. Green gap: lower efficiency for longer λ
3. Polarization fields separate electrons and holes
4. Composition fluctuations localize carriers

Can theory help?

Calculations of *functional* properties



Deslippe et al., *Comput. Phys. Commun.* 183, 1269 (2012).

Density functional theory

- Structure
- Thermodynamics
- Kinetics

GW method

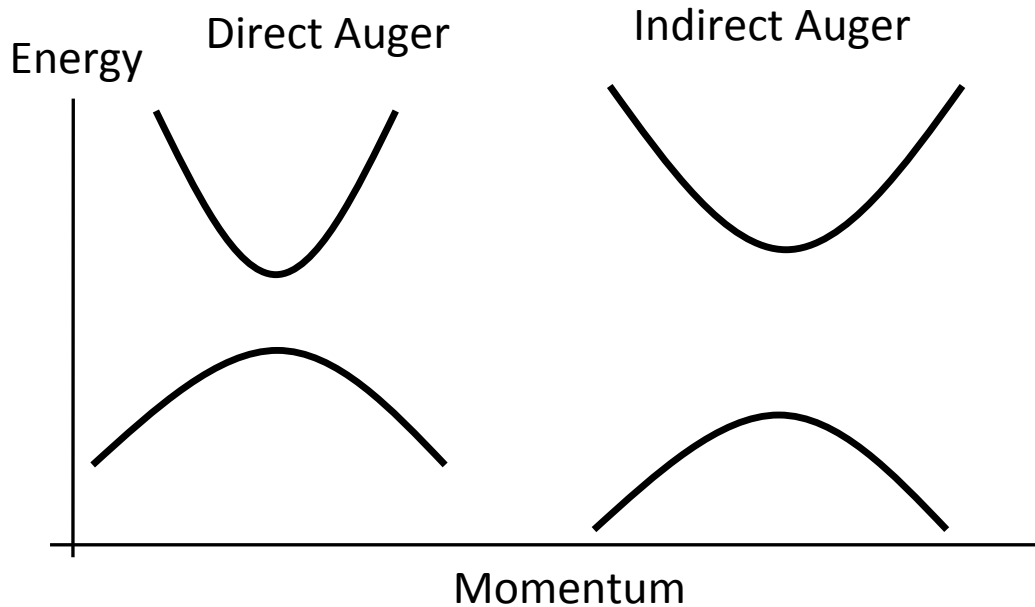
- Band gap
- Band structure

Bethe-Salpeter equation

- Light absorption/emission
- Excitons

- Combine with device simulations to model LEDs
- Microscopic understanding of efficiency problems

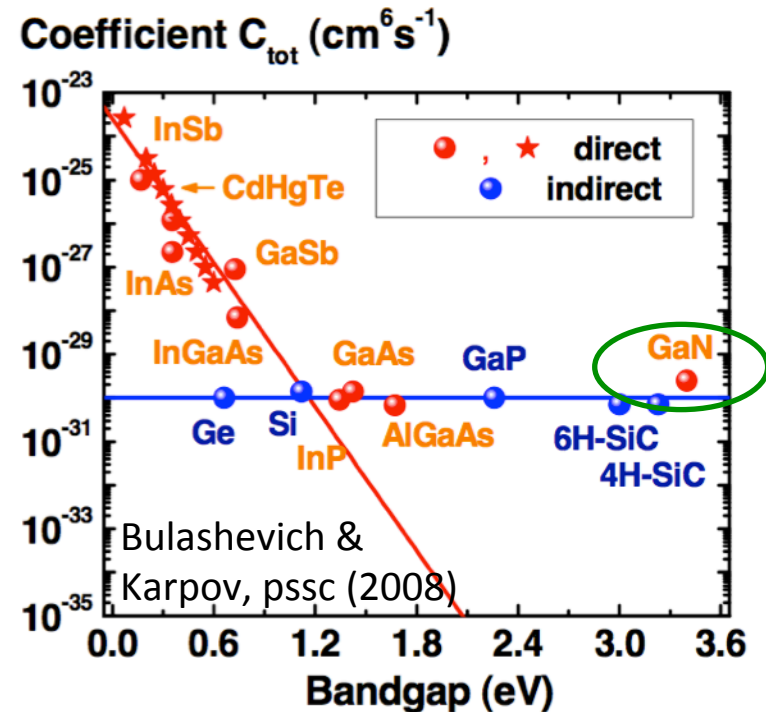
Auger recombination calculations



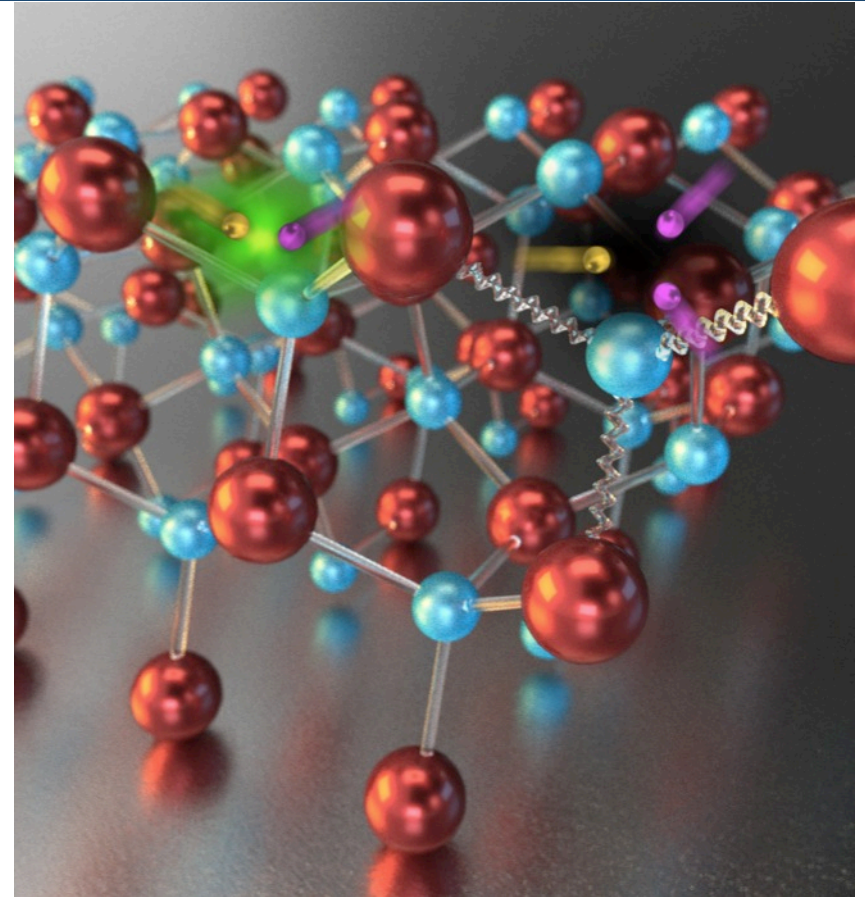
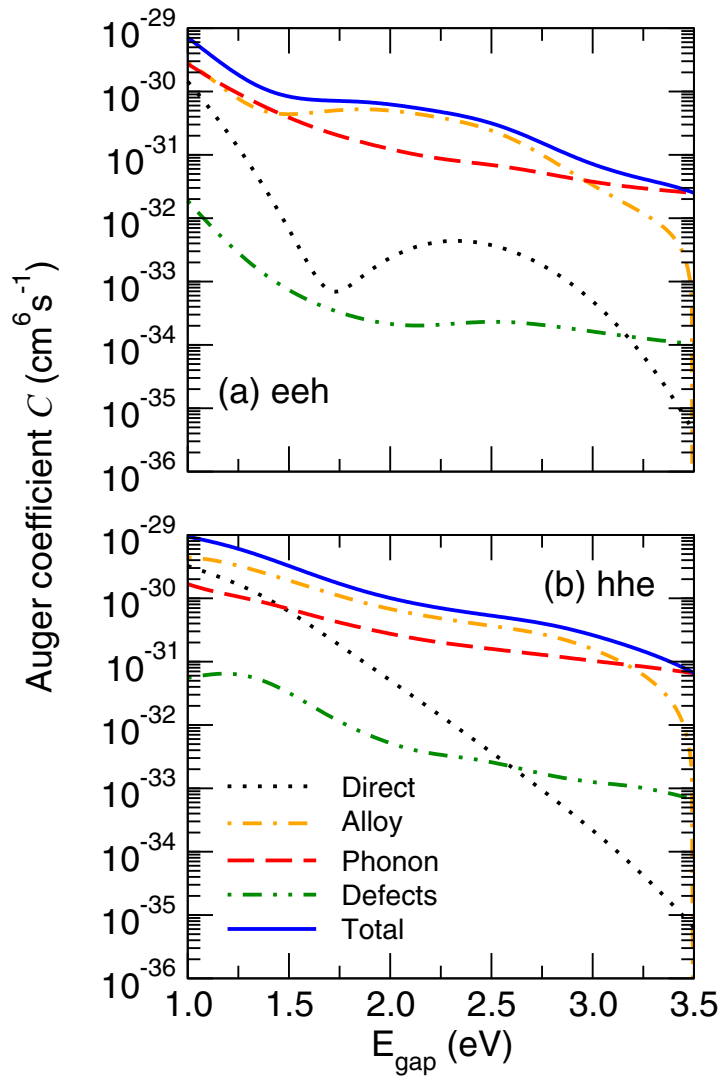
Calculations for direct Auger coefficient of GaN: $C \sim 10^{-34} \text{ cm}^6 \text{ s}^{-1}$

Too small: Experiment: $10^{-31} - 10^{-30} \text{ cm}^6 \text{ s}^{-1}$
 Hader et al., *Appl. Phys. Lett.* **92**, 261103 (2008).

But what about higher-order indirect Auger?



Indirect Auger dominates in InGaN

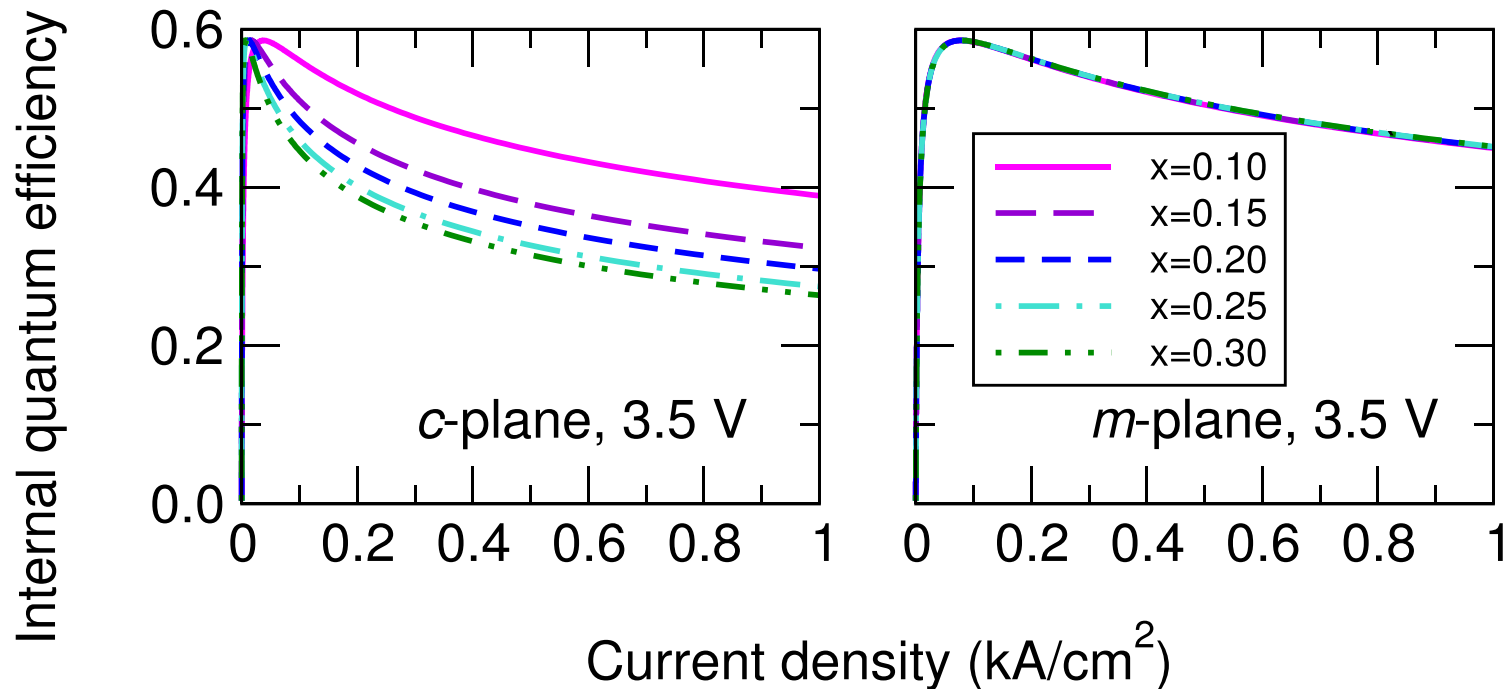


Kioupakis, Rinke, Delaney, and Van de Walle,
Appl. Phys. Lett., **98** 161107 (2011)

Kioupakis, Steiauf, Rinke, Delaney, and Van De Walle,
Phys. Rev. B **92**, 035207 (2015).

Exp: $C = 10^{-31} - 10^{-30} \text{ cm}^6 \text{ s}^{-1}$

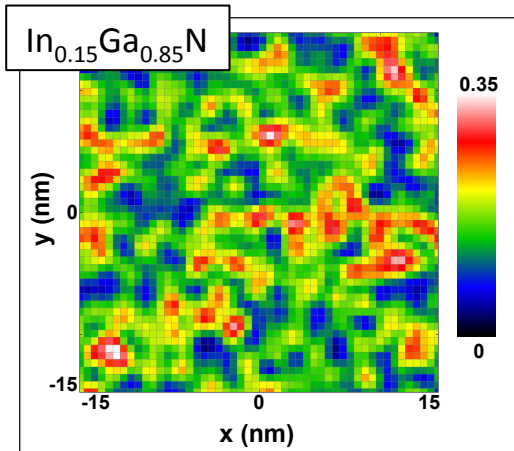
Polarization fields and droop



Green-gap problem: efficiency droop increases with increasing polarization fields, lower efficiency for LEDs at longer wavelengths

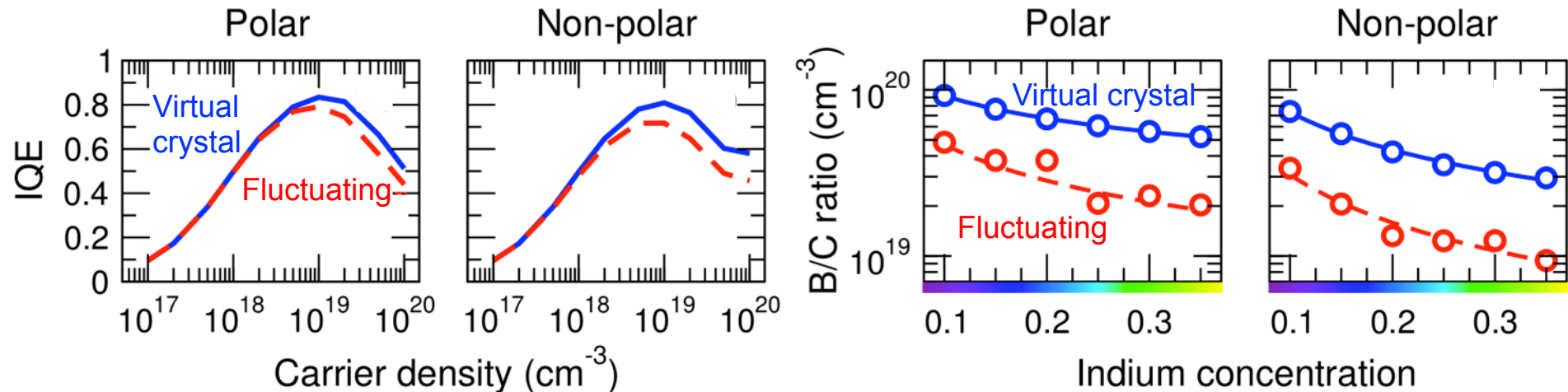
Kioupakis, Yan, and Van de Walle, *Appl. Phys. Lett.* **101**, 231107 (2012)

Fluctuations aggravate droop and green gap



Random composition fluctuations in InGaN localize electrons and holes.

- Separate electrons and holes → less overlap
- Break symmetry → enable recombination



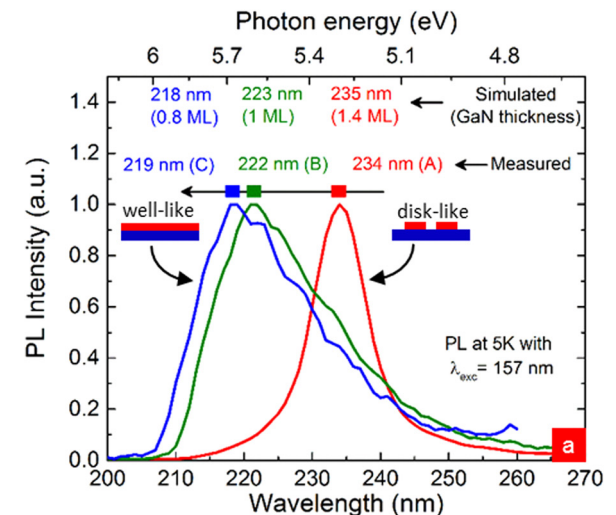
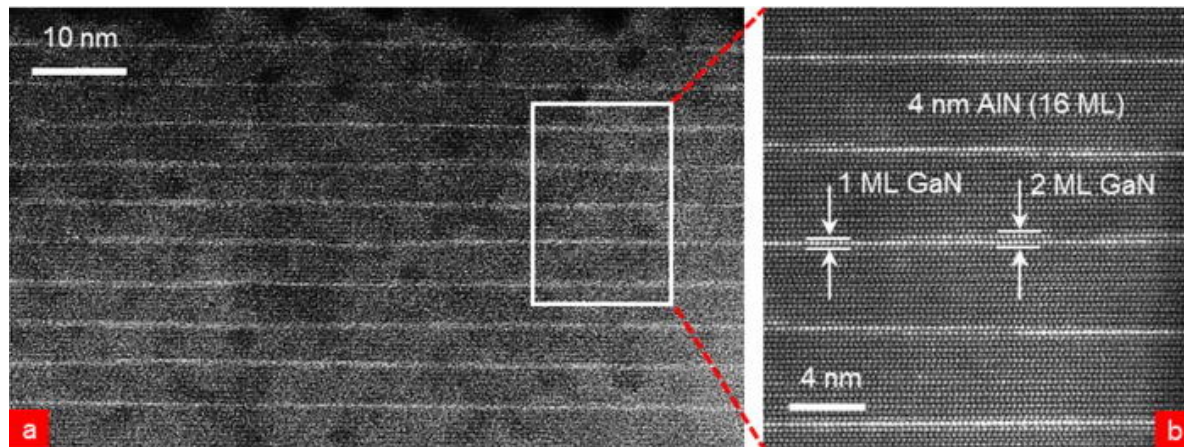
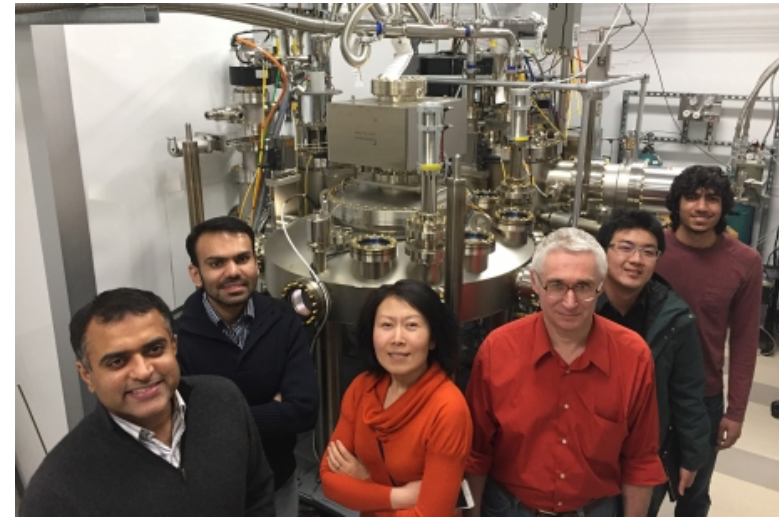
Alloy composition fluctuations *decrease* the efficiency at high power and at longer wavelengths

How to improve the efficiency?

- Auger + polarization + localization = droop + green gap.
- Unfortunately intrinsic to InGaN
- Improvements:
 - Zincblende InGaN: no polarization fields
 - *But: requires new substrates*
 - Grow more quantum wells (reduce carrier density)
 - *But: poor carrier transport*
 - Grow a single thick quantum well (reduce carrier density)
 - *But: InGaN mismatched to GaN, dislocations if too thick*
 - **Alternative: Make the quantum wells *thinner***

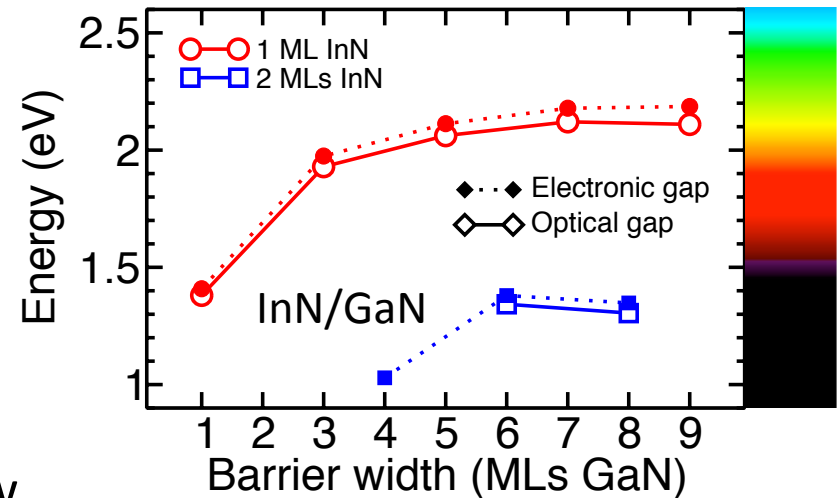
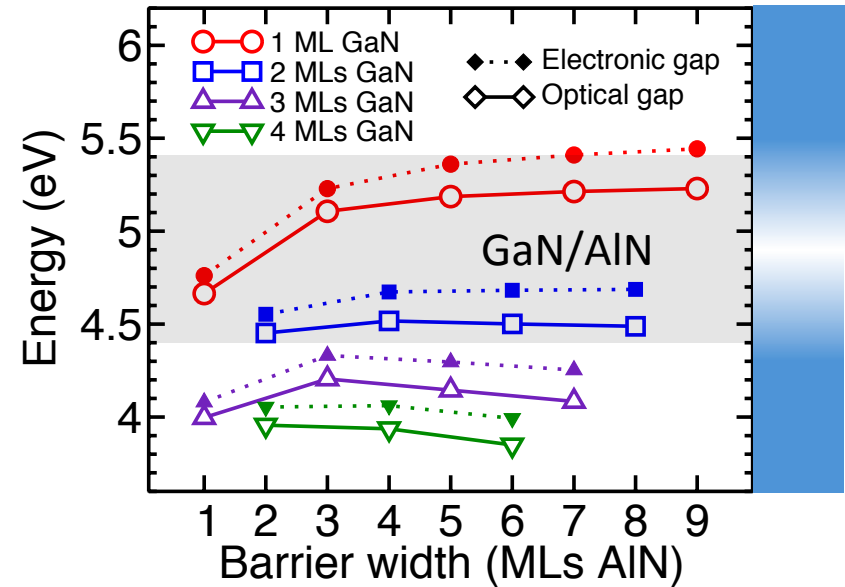
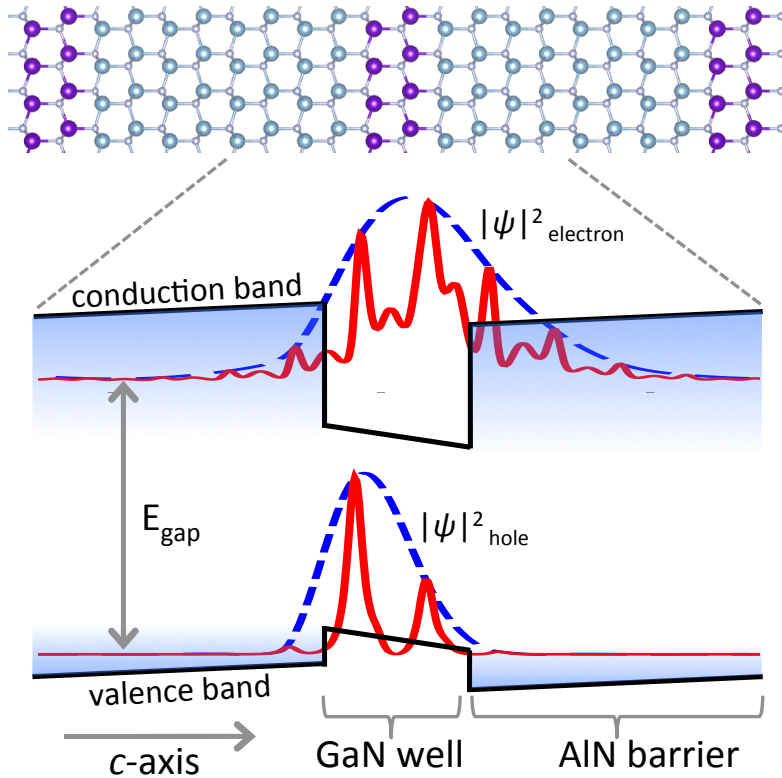
Atomically thin GaN for deep UV LEDs

- Grown by Jena and Xing at Cornell.
- Deep UV with atomically thin GaN in AlN.
- 40% IQE for deep UV emission at 219 nm



SM Islam *et al.*, Deep-UV emission at 219 nm from ultrathin MBE GaN / AlN quantum heterostructures. *Appl. Phys. Lett.* **111**, 091104 (2017).

Atomically thin quantum wells

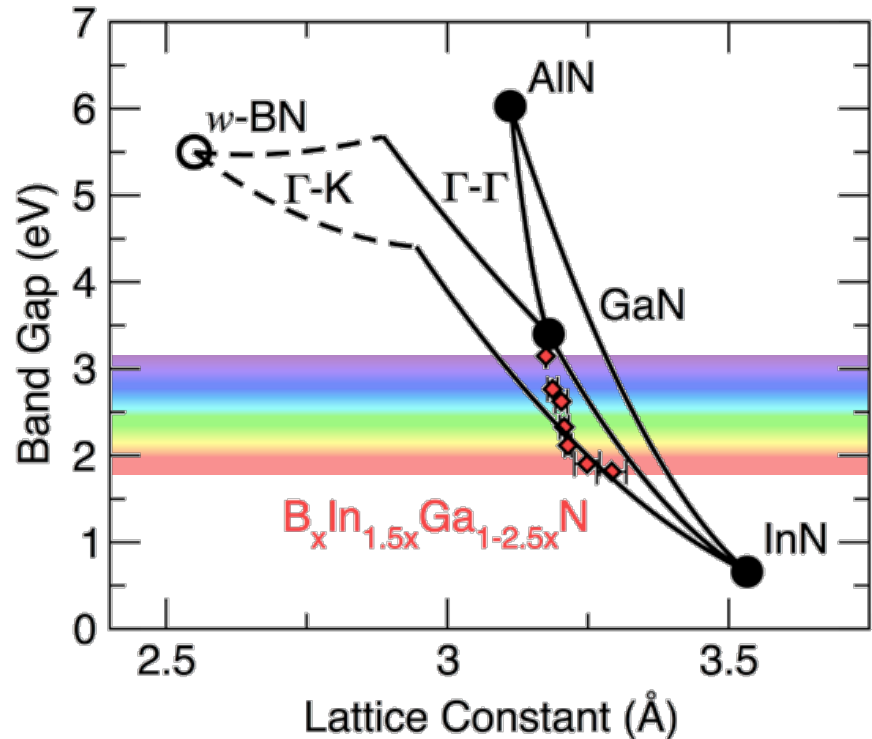
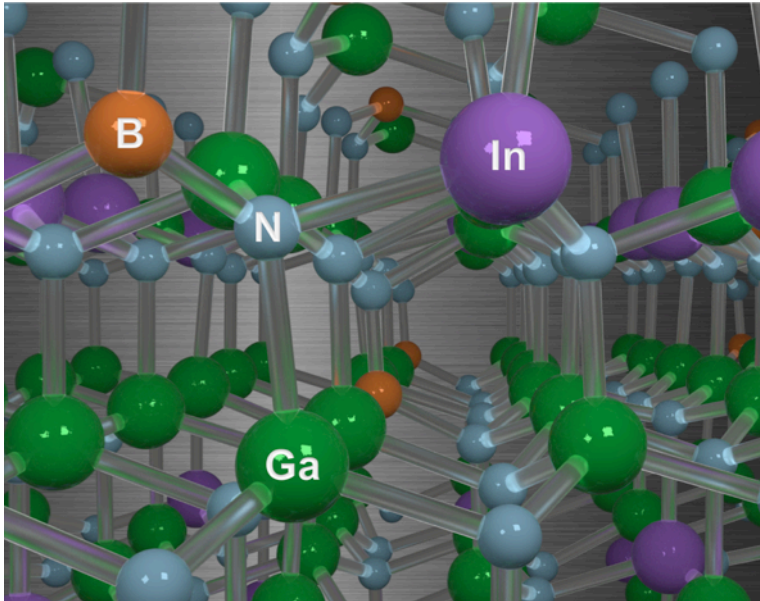


- Ordered compounds, reduced Auger
- Stark effect is weak
- Tune gap of InN in red/ amber/yellow

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BInGaN: matched to GaN, visible gap



- BInGaN alloys with a 2:3 B:In ratio are approximately lattice matched to GaN.
- Their gaps (direct) span the entire visible range.
- Increase thickness → reduce Auger.

L. Williams and E. Kioupakis, BInGaN alloys nearly lattice-matched to GaN for high-power high-efficiency visible LEDs, *Applied Physics Letters* **111**, 211107 (2017).

Perspectives for future work

- Improved emitter materials:
 - Ultrathin quantum wells
 - Boron-containing InGa(Al)N
- Collaborations with predictive theory
 - Emitters materials
 - Phosphor design
 - Thermal transport
 - Defects
 - Growth kinetics

